

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.87            | 0.81 | 0.87           | 0.82 | 0.86       | 0.86 |

Model Results

Predicted value: 7.05e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.25e-01

Confidence level: 5.69e-01

Nearest Neighbors from the Training Set

|   |  |  |
|---|--|--|
| <div>Image not found</div> <div>Asulam</div> <div>Measured: 2.17e-02</div> <div>Predicted: 7.05e-02</div> | <div>Image not found</div> <div>Methazolamide</div> <div>Measured: 1.48e-02</div> <div>Predicted: 2.36e-02</div> | <div>Image not found</div> <div>Monocrotophos</div> <div>Measured: 4.48</div> <div>Predicted: 2.47</div> |
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